What's Better, an Ensemble of Positive/Negative Pairs or a Centered Simplex Ensemble?

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INTRODUCTION

Initial perturbations of the ensemble transform Kalman filter (ETKF) ensemble forecast scheme (Wang and Bishop 2003) are independent. To center initial perturbations of the ETKF about the analysis, we can try positive/negative pairs perturbations. Theoretically, the advantage of this strategy is that the ensemble-predicted mean and covariance will be at least 3rd order accurate. Practically, for computationally expensive ensemble generation schemes such as the ECMWF singular vector ensemble (Molteni et al. 1996), it is much cheaper to generate a perturbation with an opposite sign than a new perturbation. However, for an ensemble with *K* perturbed forecasts, the 3rd order accuracy estimates by the positive/negative pairs ensemble are at most in *K*/2 directions and the remaining directions only have zero order accuracy. Besides, for computationally inexpensive ensembles such as the breeding (Toth and Kalnay,1993; 1997) and the ETKF, there is no apparent computational advantage in using positive/negative pairs. Because the true error covariance has much higher rank, to center the ETKF initial perturbations about the control analysis, we introduce a new method, called the spherical simplex ETKF. This method will yield 2nd order accurate estimates on mean and error covariance in *K*-1 directions. The goal of this paper is to answer the question "what's better, the positive/negative paired ETKF ensemble or the spherical simplex ETKF ensemble?"

THEORY OF SPHERICAL SIMPLEX ETKF

Define K forecast perturbations at the 12-h forecast lead-time as,

$$\mathbf{X}^f = (\mathbf{x}_1^f - \bar{\mathbf{x}}^f, \mathbf{x}_2^f - \bar{\mathbf{x}}^f, \cdots, \mathbf{x}_K^f - \bar{\mathbf{x}}^f), \quad (1)$$

where $\mathbf{x}_i^f$, $i = 1, \cdots, K$, are K perturbed 12-h forecasts and $\bar{\mathbf{x}}$ is the mean of the K perturbed 12-h forecasts, i.e.,

$$\bar{\mathbf{x}} = (\mathbf{x}_1 + \mathbf{x}_2 + \cdots + \mathbf{x}_K)/K. \quad (2)$$

After postmultiplying (1) by the transformation matrix $\mathbf{T} = \mathbf{C}(\mathbf{D}+\mathbf{I})^{-1/2}$ (see Bishop et al. 2001 and Wang and Bishop 2003) where **C** and **D** are the eigenvector and eigenvalue matrices of $(\mathbf{X}^f)^{\mathrm{T}}\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}\mathbf{X}^f/K$ (here **H** is the observation operator and **R** is the observation error covariance matrix), only $K-1$ independent ETKF analysis perturbations, denoted as $\mathbf{X}^a = (\mathbf{x}_1^{a'}, \mathbf{x}_2^{a'}, \cdots, \mathbf{x}_{K-1}^{a'})$, are generated.

This is because the sum of the *K* forecast perturbations in (1) is zero and therefore the last element of **D** is equal to zero. Thus, (1) postmultiplied by the last column of **C** is a zero vector. Mathematically, the $K-1$ ETKF analysis perturbations are

$$\mathbf{X}^a = \mathbf{X}^f \bar{\mathbf{C}}(\bar{\mathbf{D}}+\mathbf{I})^{-1/2}, \quad (3)$$

where $\bar{\mathbf{C}}$, a $K \times (K-1)$ matrix, contain the first $K-1$ columns of **C** and $\bar{\mathbf{D}}$ is a $(K-1)\times(K-1)$ diagonal matrix, whose diagonal elements contain the first $K-1$ eigenvalues in **D**. Note the sum of columns in $\mathbf{X}^a$ (equ. 3) is not zero and we call it one-sided ETKF initial perturbations.

The idea of the spherical simplex ETKF in centering these $K-1$ independent ETKF analysis perturbations about the control analysis at the initial time is to postmultiply $\mathbf{X}^a$ by a $(K-1)\times K$ matrix **U** to form K perturbations

$$\mathbf{Y}^a = \mathbf{X}^a\mathbf{U} = (\mathbf{y}_1^{a'}, \mathbf{y}_2^{a'}, \cdots, \mathbf{y}_K^{a'}), \quad (4)$$

where the matrix **U** is selected to ensure that a) the sum of $\mathbf{y}_i^{a'}$, $i = 1, \cdots, K$ is zero; b) the analysis error covariance associated with (3) is conserved; and c) like $\mathbf{x}_i^{a'}$, the new perturbations $\mathbf{y}_i^{a'}$, $i = 1, \cdots, K$, are equally likely. The first requirement is satisfied provided that

$$\mathbf{U}\mathbf{1} = \mathbf{0}, \quad (5)$$

where $\mathbf{0}$ is a vector with each element equal to zero and $\mathbf{1}$ is a vector with each element equal to one. The second requirement is satisfied provided that

$$\mathbf{U}\mathbf{U}^{\mathrm{T}} = \mathbf{I}, \quad (6)$$

where **I** is the identity matrix. Assuming a multi-dimensional normal distribution, then to satisfy the third requirement, the diagonal elements of $\mathbf{U}^{\mathrm{T}}\mathbf{U}$ must be equal to each other, that is, each column of **U** has the same magnitude.

So far we have found two easy solutions of **U**. Because the matrix **U** comes from the concepts of spherical simplex sigma point, we call the ETKF analysis perturbations constructed this way as the spherical simplex ETKF. One of the solutions is inherited in the ETKF transformation matrix **T**. It is easy to verify that $\bar{\mathbf{C}}^{\mathrm{T}}$ (see equ. 3) is the solution. So the K spherical simplex ETKF analysis perturbations are

$$\mathbf{Y}^a = \mathbf{X}^f \bar{\mathbf{C}}(\bar{\mathbf{D}}+\mathbf{I})^{-1/2}\bar{\mathbf{C}}^{\mathrm{T}}. \quad (7)$$

The other one is from pure geometric algebra. The experiment results for the two solutions are similar. In the following we just show those corresponding to (7).

THE INFLATION FACTOR

Because the ensemble size is much smaller than the number of directions to which the true error variance projects, the total analysis error variance is significantly underestimated by (7). So, the inflation factor method proposed in Wang and Bishop (2003) is also used in this new set of perturbations . The idea is to multiply the initial perturbations in (7) by an inflation factor to ensure that 12-h ensemble forecast variance is consistent with the 12-h control forecast error variance over global observation sites. To find this inflation factor, the maximum likelihood parameter estimation theory (Dee 1995) is used.

NUMERICAL EXPERIMENT DESIGN

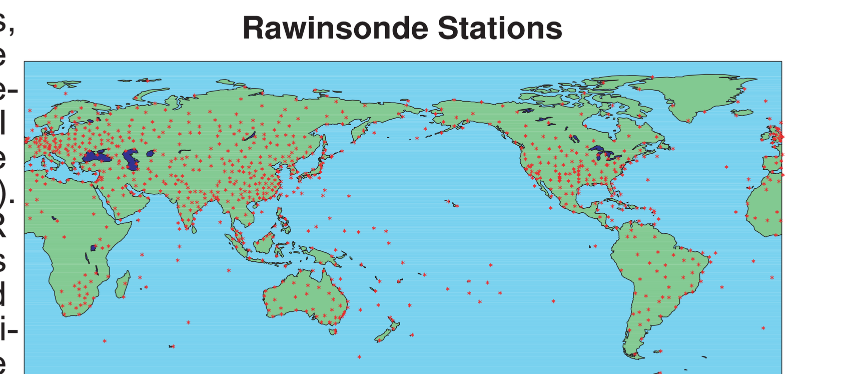

Fig. 1 Red dots denote rawinsonde stations.

We ran 17-member ensembles, one as the control forecast and the other 16 as the perturbed forecasts, i.e., K=16. The numerical model we used is version 3 of the community climate model (CCM3). We also used the NCEP/NCAR reanalysis as the control analysis and verification. The time period considered is the Northern Hemisphere summer in year 2000. The observational network is assumed to contain only rawinsonde observations (fig.1). The wind and temperature observations are assumed to take the value of the reanalysis data at the rawinsonde sites. The observation error covariance matrix is assumed to be time independent and diagonal. To estimate the observation error variance, we first calculate 12-h innovation sample variance for wind and temperature at each observation site by averaging all the squared 12-h innovations in summer of 2000 at that site. Then we choose the smallest wind and temperature innovation sample variance of all observation sites as the observation error variance.

COMPARISON RESULTS

1. Initial ensemble wind variance

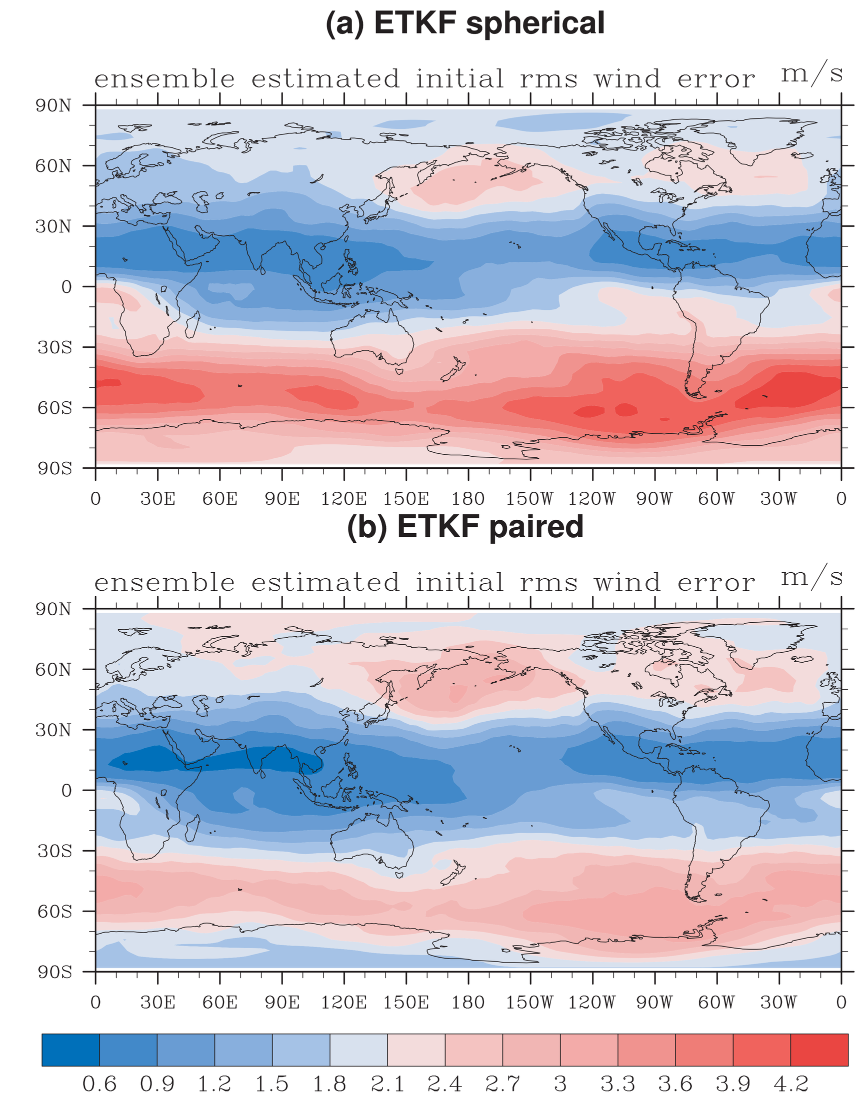

Fig. 2

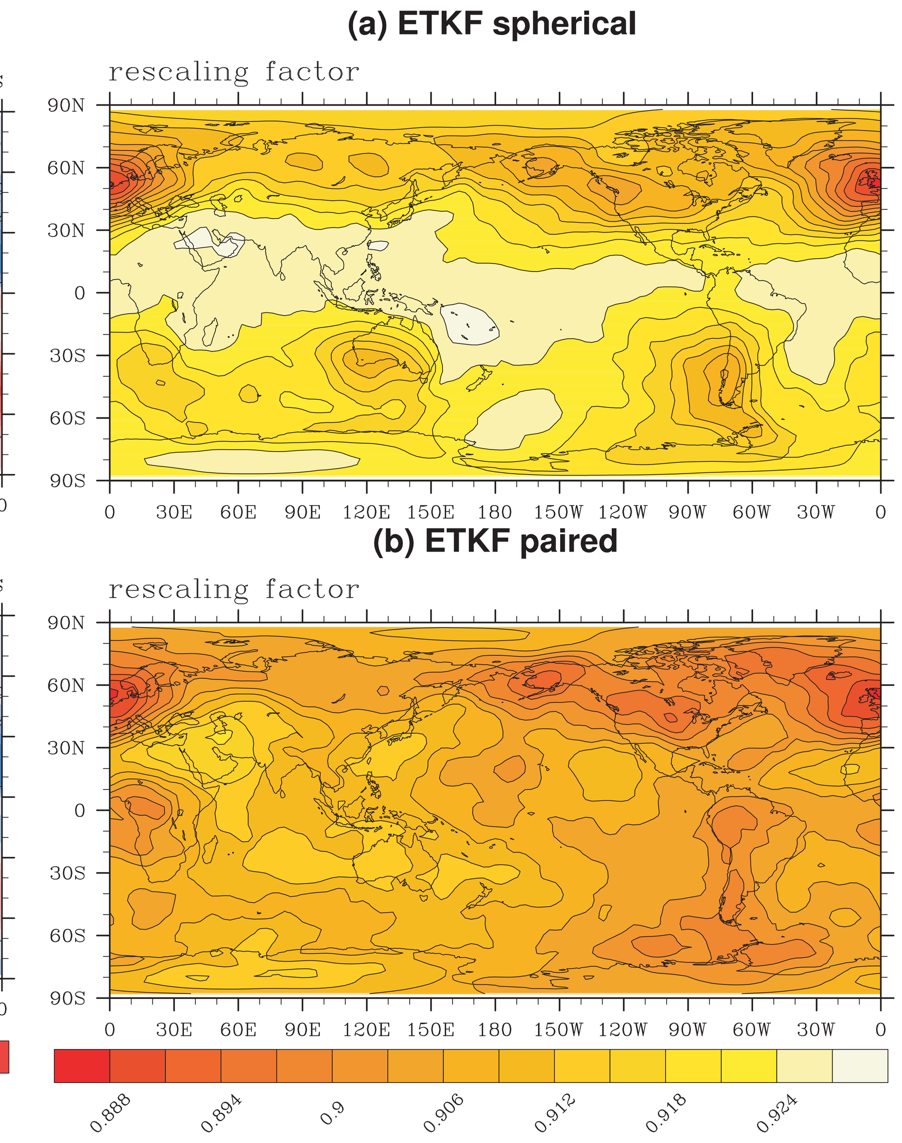

Fig. 3

To compare the performance in estimating the true error variance, we first study how the initial ensemble variance is governed by the geographical variations of observations. Fig. 2 shows the square root of the seasonally and vertically averaged initial wind error variance estimated by the spherical simplex ETKF and positive/negative paired ETKF ensembles. For both the spherical simplex ETKF and the paired ETKF ensembles, the initial ensemble variance over the ocean is larger than over the land, which is consistent with the fact that rawinsonde observation is more populated over the land. The spherical simplex ETKF initial ensemble variance (fig. 2a) over the Southern Hemisphere (SH) is much larger than over the Northern Hemisphere (NH), which reflects the fact that the rawinsonde distribution is much less distributed in the SH. However, this NH-SH contrast is much smaller for the paired ETKF (fig.2b).This result demonstrates that the spherical ETKF reflects the variation of observation density distribution to a higher degree than the paired ETKF. To better reveal how ensemble spread is governed by the observation density, we plot the rescaling factor that is defined as the ratio of ensemble-estimated initial root mean square (rms) wind error over ensemble estimated 12-h forecast rms wind error. Fig 3 shows the vertically and seasonally averaged rescaling factor. The effective rescaling factor for the spherical simplex ETKF (fig. 3a) not only reflects the high concentration of observations over Europe and North America, it is also able to account for the smaller mid-latitude observation concentrations over Southern Hemisphere (SH) continents. The rescaling factor of the positive/negative paired ETKF (fig. 3b) is only able to crudely reflect geographical variations of observations in the NH, but not for the SH.

2. Maintenance of variance along orthogonal vectors

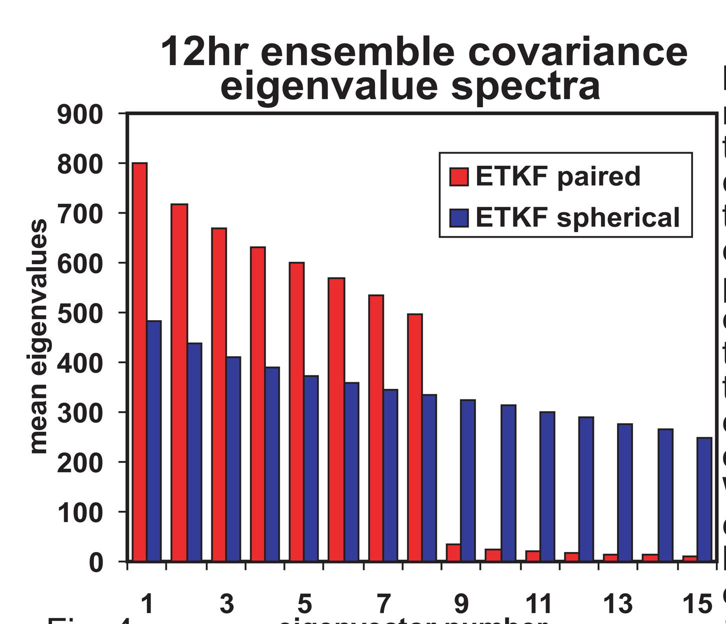

Fig. 4

For a 17-member ensemble, presumably, the error covariance estimates in predicting the true mean and true error covariance have rank of 15 for the spherical simplex ETKF ensemble, but only 8 for the positive/negative paired ETKF ensemble. This is confirmed by the averaged eigenvalue spectra for 12-h ensemble estimated error covariance matrix in observation space in figure 4. While the 12-h ensemble forecast variance for the 17-member spherical simplex ETKF ensemble is evenly spread in 15 directions, almost all ensemble variance is maintained in only 8 directions for the 17-member positive/negative paired ETKF ensemble. As a consequence, the short-term super-normal mode growth within the ensemble perturbation space is larger for the spherical simplex ETKF than for the paired ETKF (not shown).

3. Ensemble mean error

Fig. 5 shows 200-hPa, 500-hPa and 850-hPa globally averaged ensemble mean forecast error in terms of the approximate energy norm. The corresponding measurements of control forecast errors are also shown for comparison. The errors are measured against the NCEP/NCAR reanalysis data at every model grid. The ensemble mean of the spherical simplex ETKF is more accurate than the positive/negative paired ETKF and there is a bit improvement over the one-sided ETKF with the same ensemble size. Although the paired ETKF is centered on the control analysis initially, its ensemble mean is less accurate than that of the one-sided ETKF from 2 to 10-day forecast lead times.

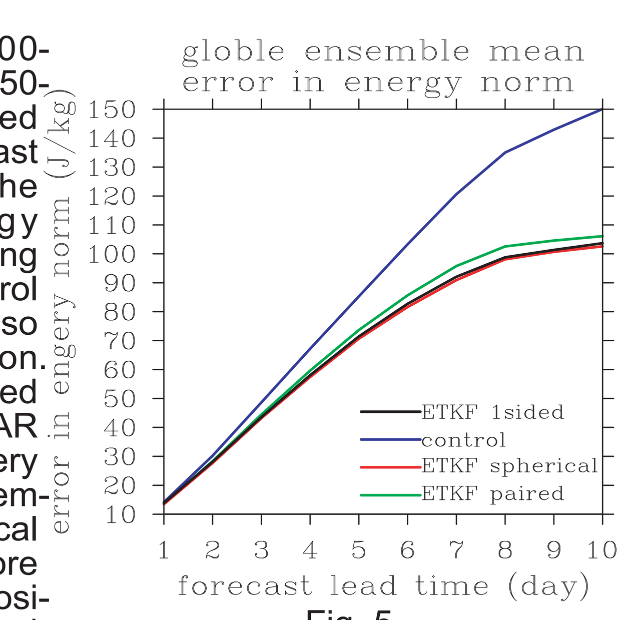

Fig. 5

4. Ensemble predictions of innovation variance

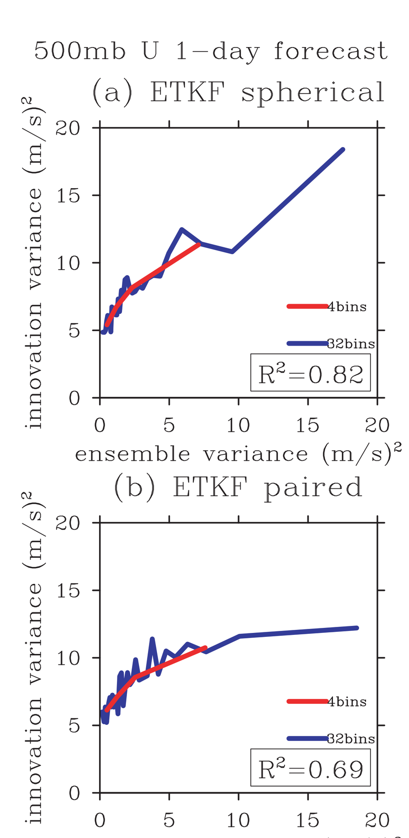

Fig. 6

Fig. 6 shows the relationship between the sample innovation variance and the ensemble variance for 500-hPa U at 1-day forecast. This figure is generated by first drawing a scattered plot for which the ordinate and abscissa of each point is respectively given by the squared 500-hPa U wind innovation and 500-hPa U wind ensemble variance at 1-day forecast at one midlatitude observation location. The innovation is defined here as the difference between the verifying analysis and the 12-h ensemble mean forecast at the rawinsonde sites. Points collected correspond to all midlatitude stations and all 1-day 500-hPa U forecast throughout the NH summer in year 2000. To begin, we divide the points into four equally populated bins, arranged in order of increasing ensemble variance. Then we average the squared innovation and ensemble variance in each bin, respectively. Connecting the averaged points then yields a curve describing the relationship between the sample innovation variance and the ensemble variance. The results corresponding to the 4-bin and 32-bin cases are shown in figure 6. First, the range of innovation variance resolved by the spherical simplex ETKF ensemble variance (fig. 6a) is much larger than that of the paired ETKF (fig. 6b). Second, as the sample size in each bin is decreased (from 4 bins to 32 bins), the relationship between sample innovation variance and the ensemble variance for 1-day forecast becomes noisier for the positive/negative paired ETKF (fig. 6b) than for the spherical simplex ETKF (fig. 6a), which is measured by the R square value. According to the analysis in section 8 of Wang and Bishop (2003), these results show that for 1-day (true for short term, e.g., 2-day not shown) forecast, the ensemble spread of the spherical simplex ETKF is more accurate in predicting the forecast error variance than that of the paired ETKF. For longer forecast lead time as 10-day (fig. 7), their skills become similar.

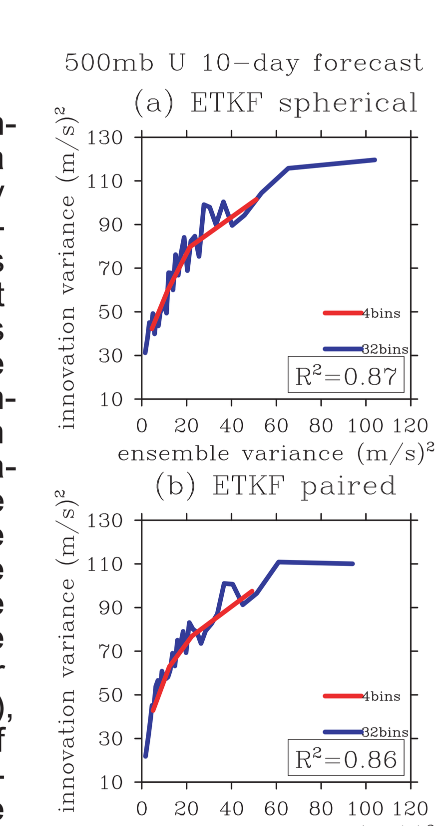

Fig. 7

SUMMARY & DISCUSSION

In this paper we compared the performance of the spherical simplex ETKF ensemble with a symmetric positive/negative paired ETKF ensemble. In the spherical simplex scheme, one more perturbation was added to the one-sided ETKF initial perturbations to satisfy a). the mean of the new set of initial perturbations equal zero, b). the covariance of the new perturbations is equal to the analysis error covariance matrix obtained from the one-sided ETKF initial perturbations, and c). all the new initial perturbations are equally likely. The spherical simplex ETKF ensemble mean was found to be more accurate than the mean of the positive/negative paired ensemble. The spherical simplex ETKF maintained comparable amounts of variance in 15 orthogonal and uncorrelated directions as compared to only 8 directions for the paired ETKF. The initial ensemble variance from the spherical simplex ETKF better reflected the geographical variations of the observations than the paired ETKF. The spherical simplex ETKF predicts forecast error variance more accurately than the paired ETKF especially for short forecast lead times.

We also tried the experiment of paired perturbations and centered single perturbations for the breeding ensembles (section 5b of Toth and Kalnay 1997) with the same experimental environment. The paired breeding has inferior forecast skill in both mean and ensemble spread than the breeding with centered single perturbations. The eigenvalue spectra (similar plot as fig. 4) of the 12-h ensemble forecast covariance matrices for the breeding with centered single perturbations are more even than the paired breeding. So both the results of the ETKF and the breeding demonstrate that given a fixed ensemble size, maintaining more rank within the ensemble perturbation subspace is more important than maintaining relatively high accuracy in small number of directions.

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